



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:26 AM UTC

PDB ID : 1IRV / pdb_00001irv
Title : CYTOCHROME C ISOZYME 1, REDUCED, MUTANT WITH ILE 75 REPLACED BY MET AND CYS 102 REPLACED BY THR
Authors : Berghuis, A.M.; Brayer, G.D.
Deposited on : 1996-06-27
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

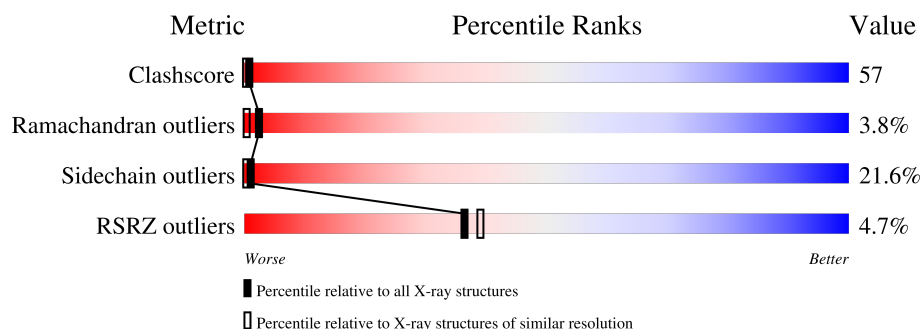
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			851	537	151	158	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	M3L	LYS	modified residue	UNP P00044
A	75	MET	ILE	engineered mutation	UNP P00044
A	102	THR	CYS	engineered mutation	UNP P00044

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

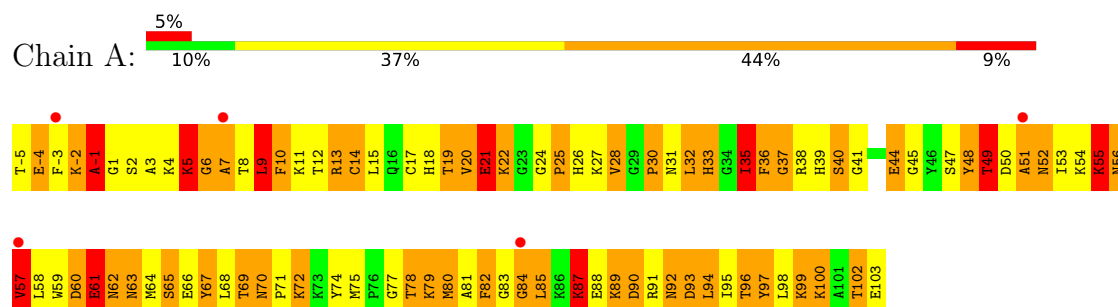
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CYTOCHROME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	36.55Å 36.55Å 138.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90 6.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (6.00-1.90) 45.3 (6.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.222 , (Not available) 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.89 , 216.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	928	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, M3L

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.72	15/857 (1.8%)	3.04	121/1146 (10.6%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	ARG	C-N	7.45	1.44	1.33
1	A	18	HIS	N-CA	7.11	1.54	1.46
1	A	96	THR	N-CA	6.77	1.54	1.46
1	A	20	VAL	C-O	6.45	1.30	1.24
1	A	28	VAL	C-N	6.23	1.42	1.33
1	A	32	LEU	C-O	6.15	1.32	1.24
1	A	90	ASP	N-CA	6.04	1.53	1.46
1	A	27	LYS	C-O	5.94	1.31	1.24
1	A	24	GLY	N-CA	5.82	1.52	1.44
1	A	69	THR	CA-CB	5.54	1.61	1.53
1	A	80	MET	CG-SD	5.43	1.94	1.80
1	A	84	GLY	N-CA	5.23	1.49	1.45
1	A	18	HIS	ND1-CE1	5.12	1.37	1.32
1	A	32	LEU	N-CA	5.08	1.52	1.46
1	A	7	ALA	N-CA	-5.00	1.40	1.46

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASN	CA-CB-CG	12.69	125.29	112.60
1	A	18	HIS	CA-CB-CG	12.01	125.81	113.80
1	A	96	THR	N-CA-C	-11.07	98.07	111.69
1	A	63	ASN	CA-CB-CG	-10.13	102.47	112.60
1	A	67	TYR	CA-C-O	-10.06	110.26	120.82
1	A	77	GLY	CA-C-N	9.90	134.76	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLY	C-N-CA	9.90	134.76	120.71
1	A	61	GLU	CA-C-N	9.77	133.72	120.44
1	A	61	GLU	C-N-CA	9.77	133.72	120.44
1	A	36	PHE	CA-CB-CG	9.49	123.29	113.80
1	A	48	TYR	CA-CB-CG	9.31	130.65	113.90
1	A	18	HIS	CA-C-N	8.97	136.90	122.81
1	A	18	HIS	C-N-CA	8.97	136.90	122.81
1	A	39	HIS	CA-CB-CG	8.89	122.69	113.80
1	A	80	MET	O-C-N	8.78	133.47	122.93
1	A	78	THR	CA-C-O	-8.63	111.69	121.19
1	A	80	MET	N-CA-CB	8.59	123.86	110.21
1	A	92	ASN	O-C-N	8.44	131.77	122.15
1	A	47	SER	CA-C-O	8.43	129.94	120.84
1	A	20	VAL	N-CA-C	8.40	121.36	112.96
1	A	28	VAL	CB-CA-C	8.26	122.28	111.70
1	A	7	ALA	O-C-N	8.24	131.59	122.11
1	A	70	ASN	CA-CB-CG	-8.19	104.41	112.60
1	A	13	ARG	CD-NE-CZ	8.18	135.86	124.40
1	A	70	ASN	OD1-CG-ND2	8.16	130.76	122.60
1	A	79	LYS	CA-C-N	-8.14	111.59	122.42
1	A	79	LYS	C-N-CA	-8.14	111.59	122.42
1	A	37	GLY	N-CA-C	-8.11	104.67	115.21
1	A	100	LYS	N-CA-CB	7.70	122.15	110.14
1	A	51	ALA	O-C-N	7.64	129.97	122.03
1	A	49	THR	N-CA-CB	7.60	123.33	110.49
1	A	87	LYS	N-CA-C	7.58	121.01	108.96
1	A	93	ASP	CB-CA-C	7.53	122.89	110.92
1	A	31	ASN	N-CA-CB	7.48	121.35	110.06
1	A	55	LYS	CA-C-N	7.47	135.81	121.54
1	A	55	LYS	C-N-CA	7.47	135.81	121.54
1	A	6	GLY	CA-C-N	7.43	131.97	120.82
1	A	6	GLY	C-N-CA	7.43	131.97	120.82
1	A	35	ILE	CA-C-O	7.18	128.78	121.17
1	A	92	ASN	OD1-CG-ND2	7.10	129.70	122.60
1	A	35	ILE	N-CA-C	7.08	117.21	110.42
1	A	57	VAL	O-C-N	7.07	130.31	122.75
1	A	62	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	15	LEU	CA-C-O	6.83	127.66	120.42
1	A	85	LEU	CA-C-O	6.76	128.40	120.70
1	A	48	TYR	CA-C-O	-6.72	113.34	120.80
1	A	61	GLU	CG-CD-OE1	6.62	133.63	118.40
1	A	10	PHE	CA-C-O	-6.61	113.50	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLU	CB-CG-CD	6.54	123.72	112.60
1	A	44	GLU	O-C-N	6.53	130.72	123.01
1	A	79	LYS	N-CA-CB	6.53	120.86	110.22
1	A	94	LEU	N-CA-C	6.52	118.93	111.11
1	A	103	GLU	CB-CA-C	-6.49	97.77	110.10
1	A	24	GLY	N-CA-C	-6.41	99.26	112.34
1	A	50	ASP	CB-CA-C	6.40	123.44	110.38
1	A	37	GLY	O-C-N	6.24	130.59	122.42
1	A	48	TYR	O-C-N	6.20	130.45	123.19
1	A	70	ASN	O-C-N	6.20	128.45	121.32
1	A	40	SER	CA-C-O	6.16	127.92	121.15
1	A	31	ASN	CA-C-O	6.10	128.00	121.05
1	A	19	THR	CA-C-N	6.06	128.69	121.84
1	A	19	THR	C-N-CA	6.06	128.69	121.84
1	A	55	LYS	CA-CB-CG	6.05	126.19	114.10
1	A	88	GLU	CG-CD-OE2	-5.97	104.68	118.40
1	A	82	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	91	ARG	CA-C-N	-5.92	111.89	120.29
1	A	91	ARG	C-N-CA	-5.92	111.89	120.29
1	A	52	ASN	OD1-CG-ND2	5.91	128.51	122.60
1	A	25	PRO	CA-C-N	-5.91	111.58	121.39
1	A	25	PRO	C-N-CA	-5.91	111.58	121.39
1	A	78	THR	CA-C-N	-5.91	111.15	122.61
1	A	78	THR	C-N-CA	-5.91	111.15	122.61
1	A	60	ASP	CA-C-O	-5.89	113.53	120.60
1	A	63	ASN	CA-C-O	5.89	127.55	121.07
1	A	26	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	33	HIS	CA-C-N	5.84	131.70	120.66
1	A	33	HIS	C-N-CA	5.84	131.70	120.66
1	A	62	ASN	CA-C-N	5.82	128.87	120.79
1	A	62	ASN	C-N-CA	5.82	128.87	120.79
1	A	51	ALA	CB-CA-C	-5.81	102.02	110.96
1	A	5	LYS	N-CA-C	-5.79	104.57	111.69
1	A	100	LYS	CA-C-O	-5.71	113.65	120.56
1	A	44	GLU	CA-CB-CG	5.69	125.49	114.10
1	A	10	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	18	HIS	O-C-N	5.68	129.85	123.48
1	A	67	TYR	O-C-N	5.66	127.90	122.07
1	A	51	ALA	N-CA-CB	5.66	118.17	109.91
1	A	10	PHE	O-C-N	5.56	128.02	122.12
1	A	91	ARG	CD-NE-CZ	-5.55	116.62	124.40
1	A	96	THR	CA-CB-CG2	5.55	119.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	TYR	CA-C-N	-5.54	116.09	122.52
1	A	74	TYR	C-N-CA	-5.54	116.09	122.52
1	A	15	LEU	N-CA-C	-5.53	105.34	111.36
1	A	21	GLU	O-C-N	5.51	129.36	122.86
1	A	30	PRO	CA-C-O	-5.50	114.39	122.31
1	A	65	SER	CA-C-O	5.48	126.41	120.55
1	A	4	LYS	N-CA-CB	5.44	119.27	110.40
1	A	50	ASP	N-CA-C	-5.44	105.37	112.23
1	A	18	HIS	CA-C-O	-5.43	114.92	120.89
1	A	7	ALA	CB-CA-C	-5.42	101.74	110.74
1	A	15	LEU	O-C-N	5.42	128.33	122.15
1	A	-4	GLU	CA-C-O	5.42	125.24	119.34
1	A	36	PHE	CB-CA-C	5.38	118.86	109.65
1	A	36	PHE	O-C-N	5.32	129.38	122.89
1	A	35	ILE	O-C-N	-5.32	116.70	121.91
1	A	97	TYR	O-C-N	5.32	127.56	122.03
1	A	56	ASN	N-CA-CB	5.29	119.42	110.49
1	A	45	GLY	O-C-N	5.22	128.56	122.45
1	A	-1	ALA	CA-C-O	5.20	127.95	120.51
1	A	69	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	103	GLU	N-CA-CB	5.18	119.31	110.50
1	A	78	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	28	VAL	N-CA-CB	-5.12	105.25	110.62
1	A	9	LEU	N-CA-C	-5.09	104.81	111.02
1	A	31	ASN	CA-C-N	-5.06	112.76	121.66
1	A	31	ASN	C-N-CA	-5.06	112.76	121.66
1	A	49	THR	OG1-CB-CG2	5.06	119.41	109.30
1	A	26	HIS	N-CA-C	-5.03	103.03	110.48
1	A	36	PHE	N-CA-CB	5.03	117.36	109.97
1	A	80	MET	CG-SD-CE	-5.03	89.84	100.90
1	A	18	HIS	CB-CA-C	-5.01	101.00	110.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	851	0	855	102	1
2	A	5	0	0	1	0
3	A	43	0	30	8	0
4	A	29	0	0	4	0
All	All	928	0	885	102	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MET:HG3	3:A:104:HEM:C1D	2.01	0.96
1:A:87:LYS:HB2	4:A:158:HOH:O	1.72	0.88
1:A:9:LEU:HD21	1:A:90:ASP:HB3	1.55	0.87
1:A:10:PHE:HB2	1:A:94:LEU:HD11	1.60	0.84
1:A:3:PHE:HB3	1:A:61:GLU:OE1	1.79	0.83
1:A:55:LYS:HG3	1:A:57:VAL:HG23	1.62	0.80
1:A:7:ALA:O	1:A:11:LYS:HE2	1.85	0.77
1:A:21:GLU:H	1:A:21:GLU:CD	1.92	0.75
1:A:5:LYS:HG2	1:A:93:ASP:HB3	1.69	0.74
1:A:80:MET:HG3	3:A:104:HEM:ND	2.04	0.72
1:A:80:MET:HE3	3:A:104:HEM:C1C	2.26	0.70
1:A:52:ASN:ND2	1:A:75:MET:HE1	2.05	0.70
1:A:5:LYS:HG2	1:A:93:ASP:CB	2.23	0.68
1:A:75:MET:SD	1:A:78:THR:HB	2.34	0.68
1:A:61:GLU:HB3	1:A:99:LYS:HE3	1.74	0.68
1:A:41:GLY:HA2	1:A:48:TYR:CZ	2.28	0.67
1:A:2:SER:HA	2:A:117:SO4:O4	1.96	0.66
1:A:7:ALA:O	1:A:11:LYS:HG2	1.96	0.66
1:A:83:GLY:HA2	4:A:172:HOH:O	1.96	0.65
1:A:94:LEU:O	1:A:97:TYR:HB3	1.97	0.65
1:A:10:PHE:HB2	1:A:94:LEU:CD1	2.27	0.64
1:A:60:ASP:OD1	1:A:63:ASN:N	2.22	0.63
1:A:41:GLY:C	1:A:48:TYR:CE2	2.77	0.62
1:A:80:MET:HE3	3:A:104:HEM:CHC	2.30	0.61
1:A:2:SER:HB3	1:A:5:LYS:HB3	1.82	0.60
1:A:10:PHE:CZ	1:A:20:VAL:HG13	2.36	0.59
1:A:95:ILE:O	1:A:99:LYS:HB2	2.02	0.59
1:A:3:PHE:CD2	1:A:61:GLU:OE1	2.55	0.58
1:A:1:GLY:O	1:A:96:THR:HG21	2.03	0.58
1:A:37:GLY:N	1:A:59:TRP:O	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:LYS:O	1:A:92:ASN:HB3	2.05	0.57
1:A:7:ALA:HA	1:A:97:TYR:CE1	2.39	0.57
1:A:41:GLY:HA2	1:A:48:TYR:CE2	2.39	0.57
1:A:5:LYS:HD3	1:A:93:ASP:OD2	2.04	0.56
1:A:67:TYR:CE2	1:A:71:PRO:HB3	2.41	0.56
1:A:8:THR:O	1:A:12:THR:HG23	2.07	0.55
1:A:79:LYS:HG2	3:A:104:HEM:HMD1	1.86	0.55
1:A:40:SER:HB3	1:A:57:VAL:HB	1.89	0.55
1:A:35:ILE:HG22	1:A:102:THR:OG1	2.06	0.55
1:A:61:GLU:HB3	1:A:99:LYS:CE	2.38	0.54
1:A:60:ASP:OD1	1:A:62:ASN:HB2	2.08	0.54
1:A:72:M3L:HE2	1:A:80:MET:O	2.08	0.53
1:A:66:GLU:O	1:A:69:THR:HB	2.07	0.53
1:A:-3:PHE:HD2	1:A:61:GLU:OE1	1.91	0.53
1:A:80:MET:HE2	1:A:82:PHE:HB3	1.91	0.53
1:A:22:LYS:HB3	1:A:33:HIS:CE1	2.44	0.53
1:A:72:M3L:HM22	1:A:81:ALA:HA	1.90	0.53
1:A:3:ALA:HB1	1:A:100:LYS:NZ	2.22	0.53
1:A:10:PHE:CD2	1:A:98:LEU:HD21	2.43	0.53
1:A:51:ALA:N	4:A:301:HOH:O	2.41	0.53
1:A:65:SER:O	1:A:69:THR:OG1	2.26	0.53
1:A:36:PHE:C	1:A:38:ARG:H	2.17	0.51
1:A:87:LYS:HB2	1:A:90:ASP:OD1	2.10	0.51
1:A:64:MET:O	1:A:68:LEU:HG	2.11	0.51
1:A:22:LYS:HB3	1:A:33:HIS:NE2	2.26	0.51
1:A:17:CYS:HB3	1:A:28:VAL:HB	1.91	0.50
1:A:75:MET:SD	4:A:166:HOH:O	2.59	0.50
1:A:7:ALA:HA	1:A:97:TYR:CD1	2.46	0.50
1:A:60:ASP:OD1	1:A:60:ASP:O	2.29	0.50
1:A:41:GLY:HA2	1:A:48:TYR:CE1	2.47	0.49
1:A:55:LYS:HG3	1:A:57:VAL:CG2	2.37	0.49
1:A:64:MET:O	1:A:64:MET:HG3	2.12	0.49
1:A:61:GLU:CB	1:A:99:LYS:HZ2	2.27	0.48
1:A:60:ASP:O	1:A:63:ASN:N	2.47	0.47
1:A:61:GLU:CD	1:A:99:LYS:HZ1	2.22	0.47
1:A:94:LEU:HG	1:A:98:LEU:CD1	2.44	0.47
1:A:13:ARG:HH11	1:A:85:LEU:CD2	2.28	0.47
1:A:6:GLY:HA3	1:A:97:TYR:HB2	1.96	0.47
1:A:82:PHE:CE1	1:A:84:GLY:HA2	2.50	0.46
1:A:72:M3L:HM32	1:A:72:M3L:HD3	1.53	0.46
1:A:5:LYS:NZ	1:A:89:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HG2	1:A:75:MET:HB3	1.98	0.46
1:A:5:LYS:HZ3	1:A:90:ASP:HA	1.81	0.45
1:A:41:GLY:CA	1:A:48:TYR:CE2	3.00	0.45
1:A:5:LYS:HG2	1:A:93:ASP:CG	2.41	0.45
1:A:14:CYS:HB3	3:A:104:HEM:C4B	2.52	0.45
1:A:61:GLU:CG	1:A:99:LYS:NZ	2.80	0.45
1:A:41:GLY:HA2	1:A:48:TYR:CD2	2.53	0.44
1:A:22:LYS:N	1:A:33:HIS:ND1	2.65	0.44
1:A:48:TYR:C	1:A:49:THR:O	2.58	0.44
1:A:-3:PHE:CZ	1:A:-1:ALA:HA	2.53	0.44
1:A:21:GLU:OE1	1:A:21:GLU:N	2.44	0.44
1:A:48:TYR:O	1:A:53:ILE:HD12	2.18	0.43
1:A:9:LEU:O	1:A:13:ARG:N	2.52	0.43
1:A:33:HIS:O	1:A:38:ARG:NH2	2.52	0.43
1:A:9:LEU:HD21	1:A:90:ASP:CB	2.39	0.43
1:A:5:LYS:HG2	1:A:93:ASP:OD2	2.19	0.43
1:A:75:MET:O	1:A:75:MET:HG3	2.18	0.42
1:A:80:MET:CG	3:A:104:HEM:ND	2.74	0.42
1:A:12:THR:C	1:A:13:ARG:HG2	2.44	0.42
1:A:32:LEU:O	1:A:35:ILE:HB	2.18	0.42
1:A:-3:PHE:HE1	1:A:92:ASN:HA	1.85	0.42
1:A:80:MET:HG3	3:A:104:HEM:CHD	2.47	0.42
1:A:5:LYS:CD	1:A:93:ASP:OD2	2.68	0.41
1:A:13:ARG:NH1	1:A:85:LEU:HD23	2.34	0.41
1:A:22:LYS:HB3	1:A:33:HIS:CD2	2.55	0.41
1:A:70:ASN:HA	1:A:71:PRO:HD2	1.81	0.41
1:A:8:THR:O	1:A:9:LEU:C	2.61	0.40
1:A:17:CYS:HB3	1:A:28:VAL:CG1	2.51	0.40
1:A:22:LYS:CB	1:A:33:HIS:CD2	3.04	0.40
1:A:19:THR:HB	1:A:21:GLU:OE2	2.20	0.40
1:A:30:PRO:HG3	1:A:48:TYR:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:CD1	1:A:62:ASN:OD1[7_555]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	105/108 (97%)	90 (86%)	11 (10%)	4 (4%)	2 0

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	61	GLU
1	A	56	ASN
1	A	-1	ALA

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/88 (100%)	69 (78%)	19 (22%)	1 0

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	THR
1	A	-4	GLU
1	A	-2	LYS
1	A	5	LYS
1	A	9	LEU
1	A	14	CYS
1	A	21	GLU

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Mol	Chain	Res	Type
1	A	22	LYS
1	A	25	PRO
1	A	35	ILE
1	A	44	GLU
1	A	54	LYS
1	A	55	LYS
1	A	57	VAL
1	A	61	GLU
1	A	87	LYS
1	A	89	LYS
1	A	99	LYS
1	A	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	42	GLN
1	A	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	M3L	A	72	1	10,11,12	0.72	0	9,14,16	1.51	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	A	72	1	-	4/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	M3L	CD-CG-CB	-2.66	103.61	113.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	72	M3L	CD-CE-NZ-CM3
1	A	72	M3L	CD-CE-NZ-CM1
1	A	72	M3L	CG-CD-CE-NZ
1	A	72	M3L	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	72	M3L	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	A	104	1	50,50,50	1.87	12 (24%)	67,82,82	1.83	13 (19%)
2	SO4	A	117	-	4,4,4	0.87	0	6,6,6	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	104	1	-	4/14/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	104	HEM	CBB-CAB	4.92	1.54	1.30
3	A	104	HEM	CBC-CAC	4.53	1.52	1.30
3	A	104	HEM	FE-NB	4.08	2.07	1.94
3	A	104	HEM	FE-ND	3.61	2.06	1.94
3	A	104	HEM	O1A-CGA	3.18	1.32	1.22
3	A	104	HEM	CMC-C2C	2.88	1.56	1.50
3	A	104	HEM	CAC-C3C	2.87	1.55	1.47
3	A	104	HEM	CMB-C2B	2.35	1.55	1.50
3	A	104	HEM	CAB-C3B	2.25	1.53	1.47
3	A	104	HEM	C3B-C2B	-2.22	1.32	1.37
3	A	104	HEM	C4A-NA	2.05	1.43	1.39
3	A	104	HEM	CBA-CGA	-2.04	1.45	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	104	HEM	CAA-CBA-CGA	8.05	135.03	113.67
3	A	104	HEM	O2A-CGA-CBA	4.74	128.99	114.00
3	A	104	HEM	CAD-CBD-CGD	4.64	125.98	113.67
3	A	104	HEM	O1A-CGA-CBA	-3.03	113.49	123.09
3	A	104	HEM	CHB-C1B-NB	2.92	127.98	124.37
3	A	104	HEM	CHC-C1C-NC	2.82	127.52	124.45
3	A	104	HEM	C1B-NB-C4B	2.59	108.27	105.21
3	A	104	HEM	CBB-CAB-C3B	-2.57	114.68	127.53
3	A	104	HEM	CHD-C1D-C2D	2.52	129.01	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	104	HEM	C4A-CHB-C1B	-2.51	120.35	126.25
3	A	104	HEM	O2A-CGA-O1A	-2.31	117.38	123.33
3	A	104	HEM	CMD-C2D-C1D	-2.19	121.61	125.03
3	A	104	HEM	C1C-CHC-C4B	-2.08	121.59	126.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

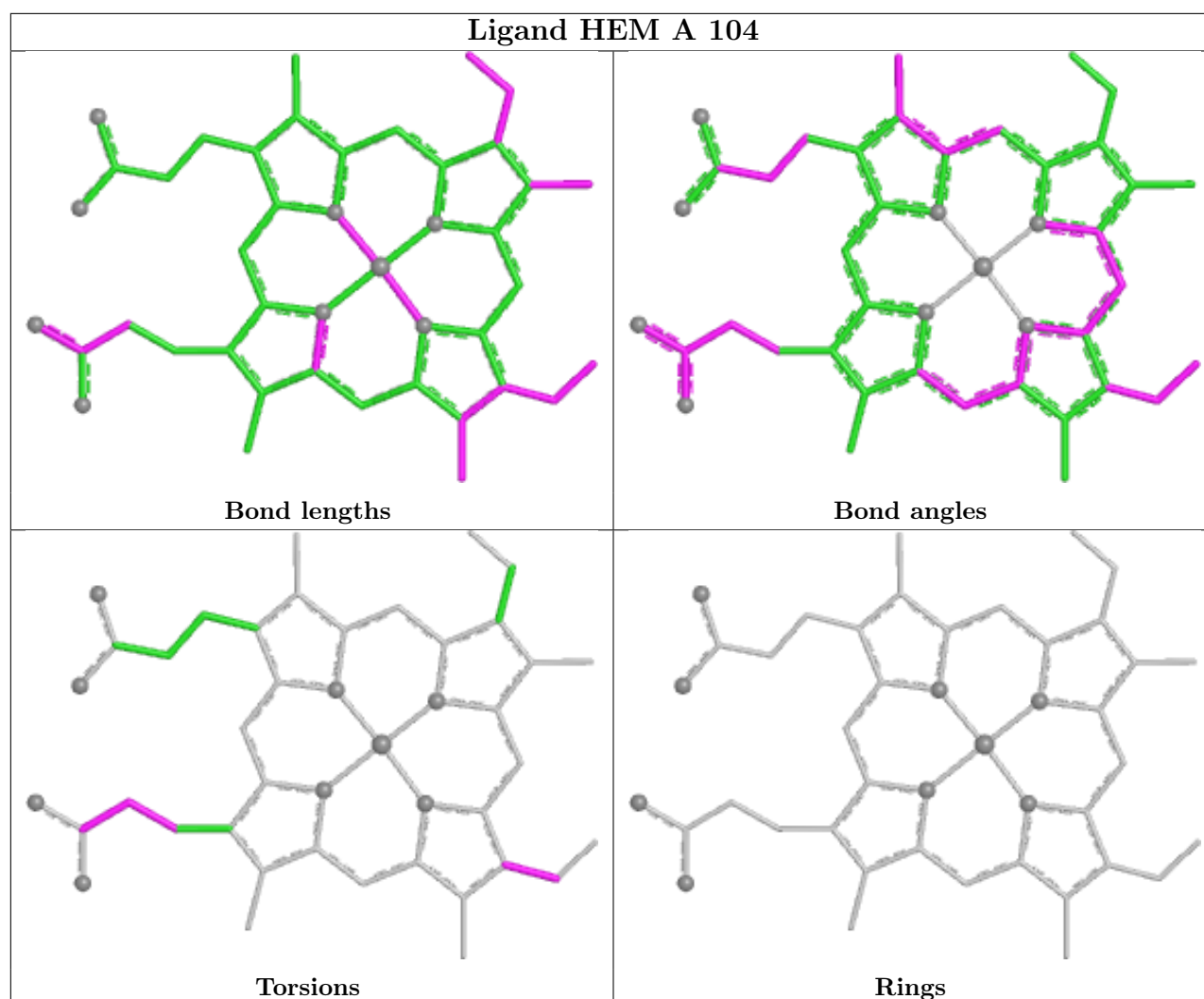
Mol	Chain	Res	Type	Atoms
3	A	104	HEM	C2B-C3B-CAB-CBB
3	A	104	HEM	C2A-CAA-CBA-CGA
3	A	104	HEM	C4B-C3B-CAB-CBB
3	A	104	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	104	HEM	8	0
2	A	117	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	107/108 (99%)	0.14	5 (4%) 36 39	4, 18, 35, 46	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	GLY	3.8
1	A	-3	PHE	3.2
1	A	51	ALA	2.3
1	A	57	VAL	2.2
1	A	7	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	M3L	A	72	12/13	0.77	0.10	12,14,18,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

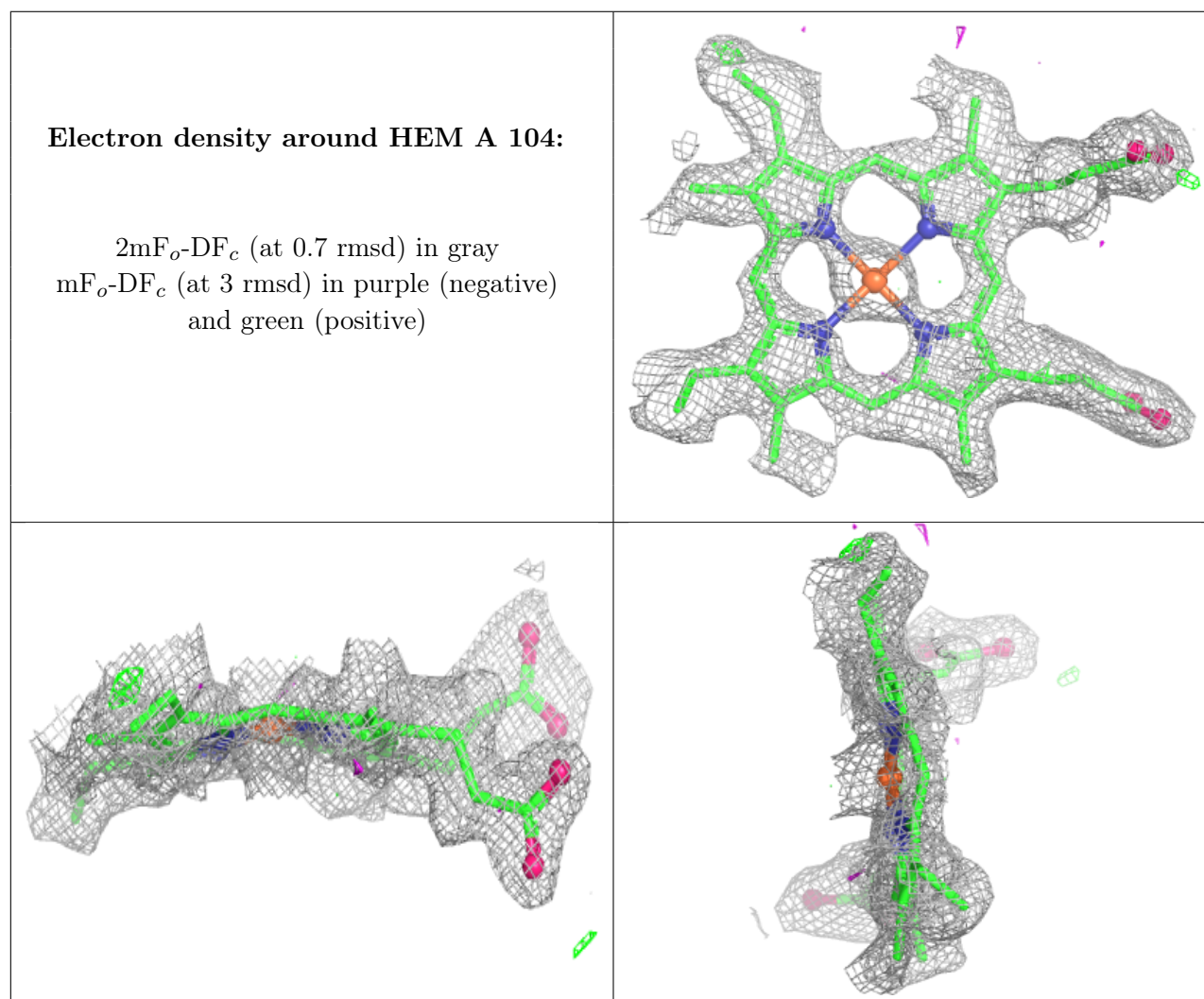
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	A	104	43/43	0.93	0.08	4,8,11,12	0
2	SO4	A	117	5/5	0.95	0.08	24,25,26,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.